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A NOTE ON THE RELATIONSHIP BETWEEN FINITE-DIFFERENCE AND SHOOTING METHODS FOR ODE EIGENVALUE PROBLEMS*

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Dedicated to Herbert B. Keller on the occasion of his 60th birthday

Abstract. Finite-difference methods and shooting methods are two standard classes of techniques for solving ordinary differential equation eigenvalue problems. We first show that a Sturm sequence method often used for solving the finite-difference eigenvalue problem may be interpreted in the shooting framework. Then we find that the Sturm sequence procedure is easily extended to more complicated problems. This enables the shooting method to guarantee convergence to specified subsets of the modes of the problem without the usual requirement of an initial guess for the eigenvalues.

Key words. shooting methods, finite-difference methods, ODE eigenvalue problems

1. Introduction. Finite-difference methods and shooting methods are two standard classes of techniques for the numerical determination of the eigenvalues and eigenfunctions of two-point boundary value problems for ordinary differential equations [1]. A typical problem is obtained from classical ocean acoustic propagation of time-periodic waves [2]. The horizontal propagation numbers λ_j and the corresponding modes $\phi_j(z)$ are the eigenvalues and eigenfunctions of

$$\phi''+\{k^2n^2(z)-\lambda^2\}\phi=0, \qquad 0<z<1, \tag{1.1a}$$

$$\phi(0)=\phi'(1)=0. \tag{1.1b}$$

In (1.1), $n^2(z)$ is the index of refraction of the stratified ocean and k is a dimensionless propagation number that depends on the frequency of the source and the depth of the ocean. The boundary conditions in (1.1) imply that the ocean's surface $z=0$ is pressure free, and that the ocean's bottom $z=1$ is rigid.

A finite-difference formulation is obtained by dividing the interval $0<z<1$ into subintervals by the mesh points $z_1, z_2, \cdots, z_N$. For an equally spaced mesh of width $h=1/N$, the mesh points are given by $z_i=ih$, $i=1,2,\cdots,N$. Then the continuous eigenvalue problem is approximated by an algebraic eigenvalue problem

$$A\boldsymbol{\phi}=\mu\boldsymbol{\phi}, \qquad \mu\equiv\lambda^2h^2, \tag{1.2}$$

where the $N\times N$ matrix A is tridiagonal if the second derivative in (1.1a) is approximated by the standard three-point difference approximation and the first derivative on (1.1b) by a two-point centered difference approximation. The N-dimensional vectors $\boldsymbol{\phi}$, with components $\phi_1, \phi_2, \cdots, \phi_N$, that are obtained from (1.2) are approximations to the eigenfunctions of (1.1) evaluated at the mesh points. Numerically determined eigenvalues μ_j and eigenvectors $\boldsymbol{\phi}_j$ of the algebraic problem (1.2) yield approximations to eigenvalues and eigenfunctions of the continuous problem (1.1).

The Sturm sequence method [3], [4] is a widely used procedure, see, for example, [5], for isolating and refining the eigenvalues of (1.2). We denote the Sturm sequence

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and ϕ' at the interface $z=1$, we get

$$A=\frac{e^{\gamma}}{2}(\phi(1)-\phi'(1)/\gamma), \qquad B=\frac{e^{\gamma}}{2}(\phi(1)+\phi'(1)/\gamma). \tag{3.3}$$

It follows from (3.2) that for λ to be an eigenvalue, $B=0$. However, for an arbitrary λ, not necessarily in the spectrum, B will not vanish in general.

It is easy to show from (3.2) and (3.3) that $\phi_f(z)$ vanishes, at most, once in the interval $(1,\infty]$. Therefore, the number of zeros of $\phi_f(z)$ in that interval is determined by comparing the signs of $\phi_f(z)$ at the endpoints. Thus, we have

$$\operatorname{sgn}\phi(\infty)=\operatorname{sgn}(B)=\operatorname{sgn}(\phi(1)+\phi'(1)/\gamma), \tag{3.4}$$

and so,

$$I(\lambda)=\text{the number of zeros of } \phi_f(z) \text{ in } (0,1] + \begin{cases} 1 & \text{if } \phi_f(1)[\phi_f(1)+\phi_f'(1)/\gamma]<0, \\ 0 & \text{if } \phi_f(1)[\phi_f(1)+\phi_f'(1)/\gamma]\geqq 0. \end{cases} \tag{3.5}$$

An impedance condition is slightly simpler if we reverse the order of integration and shoot from $z=\infty$ to $z=0$. Then the solution in $(1,\infty)$ satisfying the boundary condition at $z=\infty$ is

$$\phi_b(z)=e^{-\gamma z}. \tag{3.6}$$

This function obviously has no zeros in $(1,\infty)$. The integration is then continued numerically from $z=1$ to $z=0$ and the index function is

$$I(\lambda)=\text{the number of zeros of } \phi_b(z) \text{ in } (0,1]. \tag{3.7}$$

The above analysis is applicable to a wide class of problems. We have, for instance, developed a similar index function for optical fiber problems. There, an impedance condition is obtained at the interface of the fiber and an infinite cladding $z>1$.

4. Conclusions. We have shown that the Sturm sequence method, which is widely used for solving algebraic eigenvalue problems, can be interpreted as a shooting technique for the differential eigenvalue problem. We have also demonstrated that the bisection technique for shooting methods is generalizable to more complicated problems which have not yet been studied by traditional methods for algebraic eigenvalue problems. The extension of these techniques to higher-order problems is an important area for further research. For example, fourth-order problems arise in coupling the traditional ocean acoustic equations to an elastic ocean bottom and in fiber optics when the fourth-order vector wave formulation is used. For higher-order problems it is not clear what function is appropriate for zero counting, though in electromagnetics it has been suggested that the number of zeros in the Poynting vector is incremented with each successive mode.

Note added in proof. A similar procedure was considered in [10] for a class of nonlinear boundary value problems. However, nonlinear eigenvalue problems, infinite domains, or interpretations of Sturm's procedure for finite difference methods, which have been discussed in this paper, were not considered in [10].

corresponding to the matrix $\mu I-A$ by $S_1, S_2, \cdots, S_N$. Then $S_i(\mu)$ is the ith principal minor of this matrix, so that $S_N(\mu)$ is its characteristic polynomial. In addition, for a fixed value of μ, the number of sign changes in the sequence $\{S_i(\mu)\}$ is equal to the number of eigenvalues greater than μ (where zeros in the sequence are deleted). The sign-change property provides a simple bisection procedure for "slicing" the spectrum into isolating intervals which contain exactly one eigenvalue. The bisection procedure can be continued, or a faster root-finder such as Brent's method, can be employed to determine zeros of the characteristic polynomial $S_N(\mu)$. The root-finder should guarantee convergence to the isolated root.

An additional property of the Sturm sequence is that if $\mu=\mu_j$ is an eigenvalue, then $\phi_i=S_i$, $i=1,\cdots,N$, so that the principal minors generate the components of the eigenvectors. However, we observe that inverse iteration [3], [4] is usually employed to evaluate the eigenvectors once the eigenvalues have been determined.

In shooting methods to solve (1.1) the boundary conditions (1.1b) are replaced by initial conditions such as

$$\phi(0)=0, \qquad \phi'(0)=\alpha, \tag{1.3}$$

where α is an arbitrary nonzero constant. Then for a specified value of λ, which should be a good estimate of the desired eigenvalue λ_j, the initial value problem (1.1a) and (1.3) is numerically integrated to obtain the function $\phi(z;\lambda)$. Then the estimate of λ is improved by using a root-finder such as Newton's method, until the terminal condition $\phi'(1;\lambda)=0$ is satisfied to within some tolerance. This requires a sequence of shots with the corresponding values of λ converging to a limit, which is the shooting method approximation to the eigenvalue. The shooting method is easy to implement because accurate and efficient numerical integrators and root-finders are frequently available in subroutine libraries. However, successful applications of the method usually require accurate initial guesses for the eigenvalues, which may not be available. In addition, applications of the method may be limited by instabilities that occur when integrating into intervals in which the solution decays [6]. These instabilities may be alleviated in some cases by employing parallel shooting [1].

However, as we discuss in this paper, some aspects of the finite-difference and shooting methods for eigenvalue computation are closely related. Remarks on this relationship were previously presented in [5]. In particular, we show that the process of counting sign changes in the Sturm sequence of (1.2) is equivalent to the computation of an "index function" $I(\lambda)$ that is obtained by solving the initial value problem by a shooting method. The index function may then be employed to produce a bisection algorithm using the shooting method. This provides a systematic procedure for mode location without the requirement of an initial guess. This analysis gives a generalization of the Sturm procedure to shooting methods independent of the discretization. In addition, we extend this indexing procedure to a nonlinear eigenvalue problem that occurs in convected acoustic propagation thus generalizing the Sturm sequence procedure to the corresponding algebraic eigenvalue problem in which the eigenvalue parameter occurs nonlinearly.

Finally, we show how the present indexing may be extended to eigenvalue problems such as (1.1) where the boundary condition at $z=1$ is replaced by an impedance condition. Such impedance conditions occur, for example, in ocean acoustics where the ocean's bottom is modeled as a fluid or elastic half-space.

2. The index function. For the algebraic problem (1.2) the index function is obtained by counting sign changes in the Sturm sequence of the matrix $\mu I-A$. In addition, when μ is an eigenvalue of A, the Sturm sequence generates the eigenvectors as we have mentioned in § 1. However, when μ is not an eigenvalue the $\{\phi_i\}$ give the sequence of values that correspond to solving (1.3) by shooting, using the three-point approximation to the second derivative and the initial condition $\phi'(0)=\alpha$ such that $\phi_1=1$. Then the shooting method generates the value ϕ_i from two preceding values ϕ_{i-1} and ϕ_{i-2} by the formula

$$\phi_i=(\mu-a_i)\phi_{i-1}-\phi_{i-2}, \qquad i=2,3,\cdots,N-1, \qquad \phi_0=0, \qquad \phi_1=1, \tag{2.1a}$$

where a_i are defined for $i=1,2,\cdots,N$ by

$$a_i\equiv -2+h^2k^2n^2(z_i). \tag{2.1b}$$

Since the shooting recursions (2.1) and the Sturm sequence are identical (except at the terminal point) the Sturm method can be considered as a shooting method that employs an index function based on the number of zeros in a "trial eigenfunction" to locate a mode.

In terms of the shooting method the Sturm sequence index function is given in Theorem 1, which we now state.

THEOREM 1. *The number of eigenvalues of* (1.1) *greater than* λ *is given by the index function* $I(\lambda)$, *which is defined by*

$$I(\lambda)\equiv \text{the number of zeros of } \phi_f(z) \text{ in } (0,1]+\begin{cases}1 & \text{if } \phi_f(1)\phi_f'(1)<0,\\ 0 & \text{if } \phi_f(1)\phi_f'(1)\geqq 0.\end{cases} \tag{2.2}$$

Here $\phi_f(z)$ is the function obtained by integrating (1.1a) from $z=0$ to $z=1$ with the initial conditions $\phi_f(0)=0$ and $\phi_f'(0)=1$. The result given in Theorem 1 is stronger than the interlace property of Sturm–Liouville problem eigenfunctions because the index function is defined for values of λ that are not part of the spectrum. At a value of λ between two eigenvalues, the index function gives the number of eigenvalues greater than λ.

The proof of Theorem 1 is given in [8] for the following more general eigenvalue problem which occurs in acoustic propagation in a moving medium:

$$[\phi'/a(z,\lambda)]'+b(z,\lambda)\phi=0, \quad \phi(0)=0, \quad \phi'(1)/a(1,\lambda)=0, \tag{2.3}$$

where $a(z,\lambda)$ and $b(z,\lambda)$ are defined by

$$a(z,\lambda)\equiv[k-\lambda u(z)]^2, \qquad b(z,\lambda)\equiv n^2(z)-\frac{\lambda^2}{a(z,\lambda)}, \tag{2.4}$$

and $u(z)$ is a specified flow velocity. The analysis contained in [8] also applies to general $a(z;\lambda)$ and $b(z;\lambda)$ provided both of these functions are monotonically increasing or decreasing functions of λ within the λ-interval of interest. We observe that (2.3) is a nonlinear eigenvalue problem since the eigenvalue parameter λ occurs nonlinearly. The proof of the theorem follows from suitable comparison and oscillation theorems for ordinary differential equations, as we show in [8] and [9]. However, special attention must be given to the terminal boundary condition, as we demonstrate in § 3.

The Sturm sequence method has been extended to algebraic eigenvalue problems of the form $Ax=\lambda Bx$, where A and B are symmetric matrices and B is positive definite. To our knowledge it has not yet been extended using algebraic techniques, to eigenvalue problems which are obtained from differencing (2.3). Thus, the index function of Theorem 1 can be used to generalize Sturm sequencing to these more complicated algebraic eigenvalue problems via the shooting method.

We observe that the index function of Theorem 1 was derived for the continuous differential eigenvalue problem. However, the index function is determined numerically by shooting. Thus, sufficiently small step sizes are required in the numerical integration so that the numerical index function is calculated accurately. In actual applications "coarse" step sizes may be adequate.

The Sturm sequence method and hence the index function procedure using shooting provide stable procedures for isolating the eigenvalues. However, the resulting calculation of the eigenfunctions may be unstable, as is well known. Then the eigenvectors can be computed from the corresponding algebraic system by inverse iteration.

To make the relationship between finite-difference and shooting methods transparent we have used the same simple discretization in both approaches. In the shooting method a simple integration is used and applied directly to the second-order equations. The computational identity is preserved for the more sophisticated fourth-order Numerov's scheme which is also employed in shooting solutions of Sturm–Liouville problems. In addition, these discretizations of the second-order problem may be obtained by a discretization of an equivalent system of two first-order equations. Other implementations of the shooting method such as one employing variable step Runge–Kutta do not lend themselves to the present interpretation. However, Theorem 1 can still be used in a bisection algorithm for mode location.

3. Impedance conditions. In many physical problems the simple boundary condition $\phi'(1)=0$ inadequately describes the physics at $z=1$. More sophisticated modeling may lead to the impedance condition

$$f(\lambda)\phi(1)+g(\lambda)\phi'(1)=0, \tag{3.1}$$

where $f(\lambda)$ and $g(\lambda)$ are "prescribed" functions of the eigenvalue parameter. The differential eigenvalue problem then consists of the differential equation such as (1.1) or, more generally, the differential equation in (2.3), and the boundary conditions $\phi(0)=0$ and (3.1). In general, this eigenvalue problem and the corresponding algebraic eigenvalue problem depends nonlinearly on λ. We now show how to use the index function $I(\lambda)$ to isolate the spectrum for a special class of impedance boundary conditions, although the procedure is applicable to a more general class.

For such problems, the point $z=1$ is not a "physical" boundary, but it is an interface separating two different media. For example, in ocean acoustic wave propagation the ocean bottom $z=1$ is an interface separating the water from the sediments and rocks of the earth's mantle, which occupy the region $z>1$. This region has been modeled, for example, as an acoustic medium, an elastic medium, or as a porous elastic medium; see, for example, [7] and references given therein. For example, we consider the differential equation in (1.1a) to apply for $0<z<\infty$, such that $n(z)\equiv 1$ for $1<z<\infty$, and seek eigenfunctions which $\to 0$ as $z\to\infty$. That is, we seek to determine only the discrete spectrum of the infinite domain problem. In addition, at $z=1$, ϕ must satisfy the interfacial conditions that ϕ and ϕ' are continuous. We observe that $n(z)$ need not be continuous at $z=1$.

For an infinite domain, $I(\lambda)$ is the number of zeros of $\phi_f(z;\lambda)$ in $(0,\infty)$. We recall that the function $\phi_f(z)$ is obtained by forward integration from $z=0$ and satisfies the boundary condition at $z=0$. The number of zeros in $(0,1]$ is actually determined by a numerical integration over that interval. Since $n(z)>1$ for $z>1$, $\phi_f(z)$ is given by

$$\phi_f(z)=Ae^{-\gamma z}+Be^{\gamma z} \tag{3.2}$$

where $\gamma=\sqrt{\lambda^2-k^2}$ and $\lambda^2>k^2$ for the discrete spectrum. Requiring continuity of ϕ

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